

EUSpecLab Introductory Training School

19-30 June 2023 – RINA, Rome and UNICAM, San Benedetto del Tronto (Italy)

Programme

	Mon 19	Tue 20	Wed 21	Thu 22	Fri 23	Sat 24	Sun 25	Mon 26	Tue 27	Wed 28	Thu 29	Fri 30	
09:00			Opening/introduction to EUSpecLab (A. Trapananti/D. Sebilliau/M. Douvier)	Spin-polarised DFT and what to do with it (H. Herper)	SCIENTA Industry Day (T. Hashimoto)			Introduction to x-ray absorption spectroscopy (A. Di Cicco)	A phenomenological introduction to photoelectron spectroscopy (G. Stefan)	(K-ray) Photoelectron diffraction and related spectroscopies (D. Sebilliau)	Photoelectron spectroscopy with synchrotron radiation (M. Muntwiler)	Advanced analysis of EXAFS data using Reverse Monte Carlo and Neural Networks (F. Israr)	
			Density functional theory and its time-dependent generalization...										
10:30			coffee break	coffee break	coffee break			coffee break	coffee break	coffee break	coffee break	coffee break	
11:00	arrivals and transfer to RINA	Transfer to San Benedetto del Tronto	Density functional theory and its time-dependent generalization (M. Marques)	From theory to real-life problems: Permanent Magnets and Where to find them (A. Vishina)	SCIENTA Industry Day (T. Hashimoto)			Theory of X-ray absorption spectroscopy: introduction to core-electron spectroscopies based on the interpretation of multiple scattering approach (K. Hatada)	...photoelectron spectroscopy (G.Stefani)	Multipole interpretation of Resonant Elastic X-ray Scattering (REXS) and X-ray Absorption Spectroscopy (XAS) (S. Di Matteo)	Introduction to photo absorption and photoluminescence spectroscopies (I): phenomenology and theoretical approaches (A. Marini)	Understanding structural disorder II. Case studies (L. Pusztai)	
12:30				lunch	lunch	lunch	Social excursion to Ascoli Piceno or free time	free time	lunch	lunch	lunch	lunch	lunch
	light lunch												
14:30				Density functional theory and its time-dependent generalization (M. Marques)	An Introduction to cross sections (D. Sebilliau)	Atomic Simulation Recipes: An open Python framework for FAIR and scalable workflows (K. S. Thygesen)			Synchrotron radiation (A. Filippov)	Surface sensitivity of Electron Spectroscopy techniques: Interaction of Medium Energy Electrons with Surfaces (W. Werner)	Magnetic dichroism in x-ray spectra from a theoretician's point of view: XMCD, XMLD, XMCD, and all that jazz (D. Sipi)	Introduction to photo absorption and photoluminescence spectroscopies (II): Light emission and real-time phenomena (A. Marini)	
16:00	RINA Industry Day		coffee break	coffee break	coffee break			coffee break	coffee break	coffee break	coffee break	departures	
16:30		Welcome	Vibrational properties from density functional theory (A. Castellano)	students' talks	Atomic Simulation Recipes: remote demonstration (A. H. Larsen)			Instrumentations at Synchrotrons: a virtual tour (G. Aquilanti)	Theory of ARPES (J. Minar)	Multiple scattering description of multicolor coherent emission in photoemission and photoabsorption (C. R. Natoli)	Understanding structural disorder (in liquids and amorphous and crystalline solids) on the basis of diffraction experiments (L. Pusztai)		
18:00					students' talks				19:30 social dinner restaurant Acquapazza				

List of lectures

Wednesday 21 June

- *Density functional theory and its time-dependent generalization*
Miguel Marques Ruhr University Bochum, Germany [delivered remotely]
- *Vibrational properties from density functional theory*
Aloïs Castellano Nanomat group, CESAM, ETSF Université de Liège, Belgium

Thursday 22 June

- *Spin-polarised DFT and what to do with it*
Heike Herper, Department of Physics and Astronomy, Uppsala University, Sweden
- *From theory to real-life problems: Permanent Magnets and Where to find them*
Alena Vishina, Department of Physics and Astronomy, Uppsala University, Sweden
- *An Introduction to cross sections*
Didier Sebilliau, Univ Rennes-CNRS, IPR (Institut de Physique de Rennes), France

Friday 23 June

- *Atomic Simulation Recipes: An open Python framework for FAIR and scalable workflows*
Kristian S. Thygesen, Technical University of Denmark, Denmark [delivered remotely]
- *Atomic Simulation Recipes: remote demonstration*
Ask H. Larsen, Technical University of Denmark, Denmark [delivered remotely]

Monday 26 June

- *Introduction to X-ray absorption spectroscopy*
Andrea Di Cicco, Physics Division-School of Science and Technology, University of Camerino, Italy
- *Theory of X-ray absorption spectroscopy: introduction to core-electron spectroscopies based on the interpretation of multiple scattering approach*
Keisuke Hatada Dep. of Physics-Faculty of Science, Univ. of Toyama, Japan [delivered remotely]
- *Synchrotron Radiation*
Adriano Filipponi, Department of Physical and Chemical Sciences, University of L'Aquila, Italy
- *Instrumentations at Synchrotrons: a virtual tour*
Giuliana Aquilanti, ELETTRA-Sincrotrone Trieste, Italy

Tuesday 27 June

- *A phenomenological introduction to photoelectron spectroscopy*
Giovanni Stefani, ISM-CNR c/o Department of Science, University of Roma Tre, Italy [delivered remotely]
- *Surface sensitivity of Electron Spectroscopy techniques: Interaction of Medium Energy Electrons with Surfaces*
Wolfgang Werner, Institut für Angewandte Physik, Vienna University of Technology, Vienna, Austria
- *Theory of ARPES*
Jan Minar, University of West Bohemia, Plzeň, Czech Republic [cancelled due to health reasons]

Wednesday 28 June

- *(X-ray) Photoelectron diffraction and related spectroscopies*
Didier Sebilleau, Univ Rennes-CNRS, IPR (Institut de Physique de Rennes), France
- *Multipole interpretation of Resonant Elastic X-ray Scattering (REXS) and X-ray Absorption Spectroscopy (XAS)*
Sergio di Matteo, University of Rennes, Rennes, France [delivered remotely]
- *Magnetic dichroism in x-ray spectra from a theoretician's point of view: XMCD, XMLD, XNCD, and all that jazz*
Ondrej Sipr, FZU-Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic
- *Multiple scattering description of multicenter coherent emission in photoemission and photoabsorption*
Calogero R. Natoli, LNF-INFN, Frascati (Rome), Italy

Thursday 29 June

- *Photoelectron spectroscopy with synchrotron radiation*
Matthias Muntwiler, Paul Scherrer Institute, Villigen, Switzerland
- *Introduction to photo absorption and photoluminescence spectroscopies (I): phenomenology and theoretical approaches*
- *Introduction to photo absorption and photoluminescence spectroscopies (II): Light emission and real-time phenomena*
Andrea Marini, Material Science Institute (ISM)- CNR, Rome, Italy

- *Understanding structural disorder (in liquids and amorphous and crystalline solids) on the basis of diffraction experiments*
László Pusztai Wigner Research Centre for Physics, Budapest, Hungary

Friday 29 June

- *Advanced analysis of EXAFS data using Reverse Monte Carlo and Neural Networks*
Fabio Iesari, Aichi Synchrotron Radiation Center, Japan [delivered remotely]
- *Understanding structural disorder II. Case studies*
László Pusztai Wigner Research Centre for Physics, Budapest, Hungary